Coupling of carbon nanotubes to metallic contacts

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The modeling of carbon nanotube-metal contacts is important from both basic and applied viewpoints. For many applications, it is important to design contacts such that the transmission is dictated by intrinsic properties of the nanotube rather than by details of the contact. In this paper, we calculate the electron transmission probability from a nanotube to a free-electron metal, which is side contacted. If the metal-nanotube interface is sufficiently ordered, we find that **k**-vector conservation plays an important role in determining the coupling, with the physics depending on the area of contact, tube diameter, and chirality. The main results of this paper are (i) conductance scales with contact length, a phenomena that has been observed in experiments; (ii) in the case of uniform coupling between metal and nanotube, the threshold value of the metal Fermi wave vector (below which coupling is insignificant) depends on chirality; and (iii) an armchair tube couples better than a zigzag tube to ordered Au/Ag contacts. Disorder and small phase coherence length relax the need for **k**-vector conservation, thereby making the coupling stronger.

I. INTRODUCTION

Carbon nanotubes represent an intriguing material that has attracted much attention both from theorists and experimentalists since the early 1990s.[1] Particularly exciting is the possibility of one-dimensional metallic conductors at room temperature that can be used as a probe in scanning probe microscopy or as a low resistance ballistic interconnect for electron devices.[2–4] From a more basic point of view, much can be learned about the physics of conduction by studying the conductance of such a one-dimensional conductor at low temperatures. To exploit these possibilities it is important to understand the physics of nanotube-metal contacts, and to experimentally demonstrate low resistance contacts in a reproducible manner. The contact between carbon nanotubes and metal can occur at the end of the tube (end contact)[5,6] and along the circumference of the tube (side contact).[2,7,8] Reference 9 recently predicted interesting features in the transmission through end contacted armchair tubes. The low contact resistance demonstrated by de Pablo *et al.*[5] and Soh *et al.*[6] are due to a strong interaction between metal and carbon atoms at the end of the nanotube, or/and due to lack of translational symmetry.[10] In comparison, the interaction between metal and carbon atoms in side-contacted nanotubes is weak.

An interesting manifestation of weak distributed coupling is that the contact resistance is inversely proportional to the contact length, as observed experimentally in Refs. 2 and 8. Recently Tersoff, in a perceptive paper,[10] qualitatively discussed the importance of **k**-vector conservation when the coupling between nanotube and metal is weak. The important physical quantities are the diameter and chirality of the nanotube, the Fermi wave vector of the metal, area of contact, and details of the metal-nanotube contact. In this paper, we study the physics of side-contacted nanotube-metal contacts[2,8] by addressing how these physical quantities affect the transmission of electrons from the nanotube to the metal contact. For small diameter nanotubes, our conclusions do not fully agree with Ref. 10. We find that for small diameter armchair tubes, the threshold value of the Fermi wave vector below which the conductance is very small is $2\pi/3a_0$ and not $4\pi/3a_0$, which is the threshold value for graphene. $a_0 = 2.46$ Å is the lattice vector length of graphene. In contrast to armchair tubes, the threshold for zigzag tubes is zero. Our calculations also show that the conductance scales with contact length, a phenomenon that was observed experimentally in the work of Tans *et al.*[2] and Frank *et al.*[8]

In the remainder of the introduction, we discuss the salient results using simple arguments. The method is discussed in Sec. II, and the numerical results and discussion are presented in Sec. III. We present our conclusions in Sec. IV.

The first Brillouin zone of graphene touches the Fermi surface at six points (Fig. 1). Of these, only two points are inequivalent (that is, do not differ by a reciprocal-lattice vector). The conduction properties of graphite at a low bias are controlled by the nature of eigenstates around these points. Consider a metal making uniform contact to graphene. The in-plane wave vector should be conserved when an electron

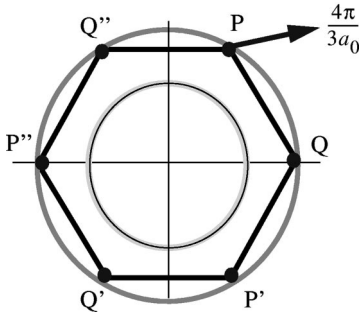

FIG. 1. First Brillouin zone of graphene. Points P, P', P'', Q, Q', and Q'' touch the Fermi surface. a_0 is the lattice vector length of graphene. A metal with a Fermi wave vector smaller (inner circle) and larger (outer circle) than $4\pi/3a_0$ couples poorly and well to graphene, respectively.

tunnels from the metal to the nanotube. As a result, for good coupling between metal and graphene, the metal Fermi wave vector should be comparable to $4\pi/3a_0$, which corresponds to the Fermi wave vector of graphene.

To discuss the case of nanotubes making contact to metal, we consider the scattering rate $(1/\tau_{c-m})$ from the metal to nanotube within the Born approximation,

$$1/\tau_{c\text{-}m} \propto \langle \Psi_c | H_{c-m} | \Psi_m \rangle, \tag{1}$$

where $\Psi_m(\Psi_c)$ is the metal (nanotube) wave function and $H_{c\text{-}m}$ represents the nanotube-metal coupling. The wave function of an (n,m) nanotube is $\Psi_c \sim e^{ik_t pu}\phi_c$, where k_t is the axial wave vector, u is the one-dimensional unit cell length, p is an integer representing the various unit cells, and ϕ_c is a vector representing the wave function of all atoms in a unit cell. It is assumed that the wave function of the metal is separable in the axial and radial directions of the nanotube, $|\Psi_m\rangle \sim e^{ik_m pu}|\phi_m\rangle$, where k_m is the metal wave-vector component along the nanotube axis. When the coupling between the nanotube and metal is uniform, the scattering rate is [Eq. (1)]

$$1/\tau_{c\text{-}m} \propto t_{c\text{-}m}\langle \phi_c | \phi_m \rangle \sum_p e^{i(k_m - k_t)pu}, \tag{2}$$

where the summation is performed over all unit cells making contact to metal, and $t_{c\text{-}m}$ represents a uniform coupling constant between the metal and nanotube. It is clear from Eq. (2) that provided the metal and nanotube make contact over several unit cells, wave-vector conservation along the axial direction is enforced as $\Sigma_p e^{i(k_m-k_t)pu} \sim (1/u)\,\delta(k_m - k_t)$. The axial wave vector corresponding to $E=0$ are $2\pi/3a_0$ and 0 for armchair and zigzag tubes, respectively, and the wave vector for other chiralities varies between these two limits. As a result, the threshold value of the Fermi wave vector, below which the coupling between an armchair (zigzag) nanotube and metal is poor, is equal to $2\pi/3a_0(0)$. The threshold value of the metal Fermi wave vector for chiral tubes is in between that of zigzag and armchair tubes. As the diameter of the nanotube increases, wave-vector conservation along the circumference becomes increasingly important, as the graphene strip approaches a graphene sheet.

II. METHOD

The method used to calculate transmission probability is essentially the same as that in Ref. 4, with the only addition being the connection of a metal contact.[11] So in this section, we mainly focus on the connection to the metal contact. The metal contact has a rectangular cross section in the (x,z) plane and is infinitely long along the y axis, as shown in Fig. 2. The nanotube lies on the metal contact akin to the experiment of Tans *et al.*[2] In Ref. 2, the nanotube bends over the edge of the metal, and the influence of this on transport was recently modeled by Rochefort *et al.*[12] In this work, the main focus is to model the coupling between the metal and nanotube. So we assume the nanotube to lie rigidly on the metal, and neglect the effect of bending (Fig. 2). A perfectly cylindrical nanotube would touch the metal surface only along a line. To simplify modeling this interface, we stretch the entire circumference of the nanotube over the metal surface,

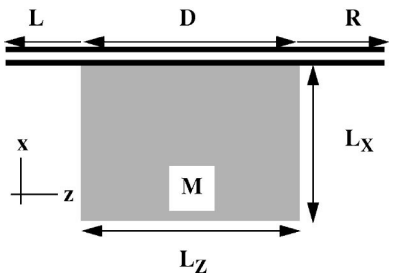

FIG. 2. A metal making contact to a nanotube. The (x,z) dimensions of the metal form a rectangular cross section with lengths (L_x, L_z). The y direction is infinitely long.

and assume coupling between carbon atoms in a sector of the circumference and the metal; the Hamiltonian of the nanotube is assumed to be the usual one for a circular tube. Finally, charge self-consistency[13] has been neglected.

The transmission and local density of states are calculated in a structure that can be conceptually divided into four parts: the section of the nanotube (D), which lies on the metal electrode (M), and semi-infinite regions L and R of the nanotube (Fig. 2). The Hamiltonians of the system can be written as

$$H = H_c + H_m + H_{c\text{-}m}, \tag{3}$$

$$H_c = H_D + H_L + H_R + H_{LD} + H_{RD}, \tag{4}$$

where H_c is the pi-electron tight-binding Hamiltonian of the nanotube with the on-site potential and the hopping parameter between nearest-neighbor carbon atoms equal to 0 and 3.1 eV, respectively.[1] H_{LD} and H_{RD} are terms in the Hamiltonian coupling D to L and R, respectively. H_m and $H_{c\text{-}m}$ are the free-particle and nanotube-metal coupling terms of the Hamiltonian. The Green's function G^r is obtained by solving $[E - H_D - \Sigma_L^r - \Sigma_R^r - \Sigma_m^r]G^r(E) = I$, where the self-energy $\Sigma_\alpha = V_{D\alpha} g_\alpha^r V_{\alpha D}$ ($\alpha \in L, R$, and M). g_α^r is the surface Green's function of lead α and $V_{D\alpha}(V_{\alpha D})$ is the coupling between $D(\alpha)$ and $\alpha(D)$. The transmission probability between leads α and β $[T_{\alpha\beta}]$ is given by

$$T_{\alpha\beta}(E) = \mathrm{Tr}[\Gamma_\alpha(E) G^r(E) \Gamma_\beta(E) G^a(E)], \tag{5}$$

where $\Gamma_\alpha(E) = 2\pi V_{D\alpha}\rho_\alpha(E) V_{\alpha D}$, and $\rho_\alpha(E) = -(1/\pi)\mathrm{Im}[g_\alpha^r(E)]$ is the surface density of states of lead α.

The Green's function of the metal contact is calculated within the free-electron approximation using the procedure outlined below. The metal contact has a rectangular cross section of dimensions L_x and L_z in the x and z directions, respectively, and is infinitely long in the y direction. While the (y,z) coordinates are assumed to be continuous, the x coordinate is assumed to be discrete with lattice spacing $a = L_x/(N_x+1)$, where N_x is the number of lattice points. The wave functions (Ψ_{mkn}) and eigenvalues (E_{mkn}) are given by

$$\Psi_{mkn}(r) = X_m(x) Y_k(y) Z_n(z), \tag{6}$$

where

$$X_m(x) = \frac{1}{\sqrt{L_x}} \sin\left(\frac{m\pi x}{L_x}\right), \quad Y_k(y) = \frac{1}{\sqrt{L_y}} \exp(iky),$$

$$Z_n(z)=\frac{1}{\sqrt{L_z}}\sin\left(\frac{m\pi z}{L_z}\right),$$

$$E_{mkn}=\frac{\hbar^2}{2m_o a^2}\left[1-\cos\left(\frac{m\pi}{N_x+1}\right)\right]+\frac{\hbar^2 k^2}{2m_o}+\frac{\hbar^2}{2m_o}\left(\frac{n\pi}{L_z}\right)^2, \tag{7}$$

where m and n are positive integers, and m_0 is the free-electron mass. Using Eqs. (6) and (7) in the equation for the Green's function,

$$g(r,r',E)=\sum_{m,k,n}\frac{\Psi_{mkn}(r)^*\Psi_{mkn}(r')}{E-E_{mkn}+i\eta},$$

we obtain,

$$g(r,r',E)=-\frac{im_o}{\hbar^2}\frac{1}{L_x L_z}\sum_{m,n}\frac{\exp[ik_I|y-y'|]}{k_I}\times\sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{m\pi x'}{L_x}\right)\sin\left(\frac{n\pi z}{L_z}\right)\sin\left(\frac{n\pi z'}{L_z}\right), \tag{8}$$

where,

$$k_I=\left\{k^2-\left(\frac{n\pi}{L_z}\right)^2-\frac{1}{a^2}\left[1-\cos\left(\frac{m\pi}{N_x+1}\right)\right]+i\eta\right\}^{1/2} \quad \text{and}$$

$$k=\sqrt{\frac{2m_o E}{\hbar^2}}. \tag{9}$$

For carbon nanotubes, the zero of energy ($E=0$) is taken to lie at the band center. On the other hand, in deriving Eq. (8) the zero of energy corresponded to the band bottom of the free-electron metal. In the calculations, there should be only one zero of energy, which we take to lie at the band center of the nanotube. We also neglect charging effects, and assume the Fermi energy of the metal to lie at the band center of the nanotube.[14] Then, in the coordinate system where $E=0$ corresponds to the band center of the nanotube, Eq. (8) can be used by transforming,

$$k=\sqrt{\frac{2m_o E}{\hbar^2}} \quad \text{to} \quad k=\sqrt{\frac{2m_o E}{\hbar^2}+k_f^2}$$

in Eq. (9), where k_f is the Fermi wave vector of the metal.

The component of the Green's function that enters the calculation of the density of states and transmission probability corresponds to $x=x'=a$, the surface of the metal contact on which the nanotube lies. The (y,z) coordinates correspond to the atomic location of the stretched out nanotube lying on the metal. For uniform coupling between the metal and nanotube, we take $V_{DM}=tD_0$, where t is the strength of coupling between the free-electron metal and a nanotube atom, and D_0 is a diagonal matrix whose dimension is equal to the number of carbon atoms in D. The diagonal entry $D_0(i,i)=1(0)$ if the carbon atom ''i'' makes (does not make) contact to the metal.

TABLE I. Γ_M for the different values of the metal Fermi wave vectors used.

Metal Fermi wave vector (Å^{-1})	Γ_M(eV)
0.4	1.1×10^{-4}
0.75	7.2×10^{-4}
0.9	1.2×10^{-3}
1.2	2.9×10^{-3}
1.75	9.1×10^{-3}

III. RESULTS AND DISCUSSION

We first present results for the dependence of the threshold value of the metal Fermi wave vector on chirality, using armchair and zigzag tubes connected to the metal contact. We then discuss the diameter dependence of the conductance, using the case of a zigzag tube as an example. Finally, the case of disorder in coupling between a nanotube and metal is considered. We consider only weak coupling between the nanotube and metal. The average value of the nonzero diagonal elements of the coupling strength Γ_M are tabulated in Table I for the various values of the metal Fermi wave vector considered. The main guide for the choice of Γ_M is that it be much smaller than the corresponding coupling strength between two carbon atoms of the nanotube [the diagonal component of Γ_L is approximately equal to

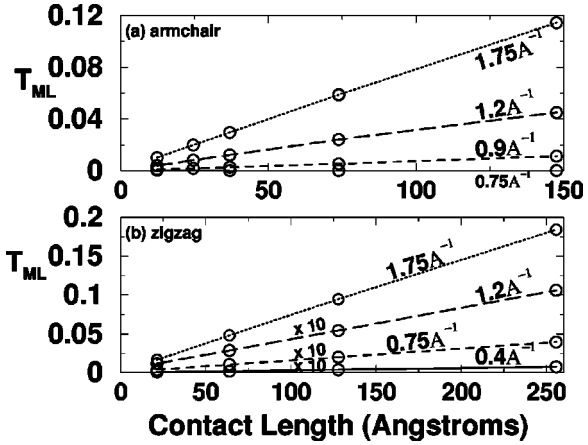

FIG. 3. Transmission probability for (a) armchair and (b) zigzag tubes vs the contact length. In both cases the largest contact length corresponds to 60 unit cells. The main point of (a) is that for the metal Fermi wave vector smaller than the threshold $2\pi/3a_0$, coupling between the nanotube and metal is small, and increasing the contact length does not change the transmission probability. For a metal Fermi wave vector larger than $2\pi/3a_0$, the transmission probability increases with an increase in the contact length and also with an increase in k_f for a given contact length. The main point of (b) is that there is no threshold in the metal Fermi wave vector. Even in the case of a small value of the metal Fermi wave vector (0.4 Å^{-1}), the transmission increases with an increase in the contact length, though the magnitude of transmission is small. As in the armchair case, the transmission probability increases with an increase in k_f for a given contact length. Values of T_{ML} in (b) corresponding to k_f equal to 0.4, 0.75, and 1.2 Å are multiplied by a factor of 10.

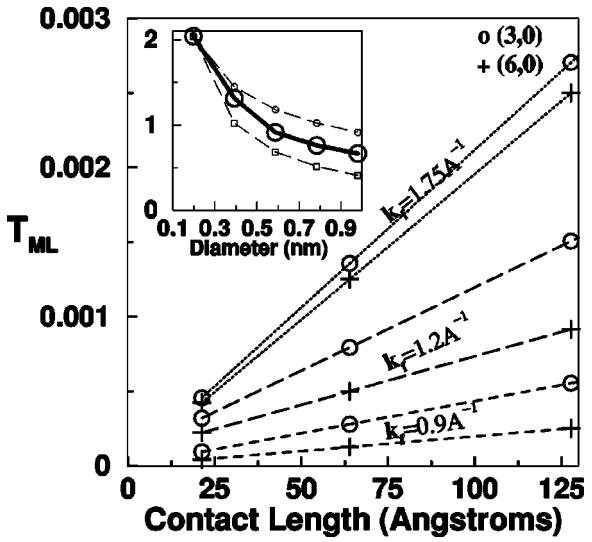

FIG. 4. Comparison of the transmission probability of (3,0) and (6,0) nanotubes vs the contact length. The transmission probability decreases with an increase in the diameter. Inset: The y axis is T_{ML} for metallic zigzag tubes scaled by $1.0e+4$. The solid line is the diameter dependence of T_{ML} for a contact length of 42.6 Å. The upper and lower dashed lines are $1/\sqrt{\text{diameter}}$ and 1/diameter dependences, shown for comparison.

$0.3eV$ for a (2,2) nanotube]. A larger (smaller) value of Γ_M will result in a larger or smaller value of transmission in Figs. 3–5. We calculate the transmission versus contact length between the nanotube and metal for various Fermi wave vectors in the metal, and all atoms around the circumference of the tube are assumed to make uniform contact with the metal. We emphasize that when the metal makes contact with only a sector of the nanotube such as in Ref. 2, the results of the Fermi wave-vector dependence on chirality

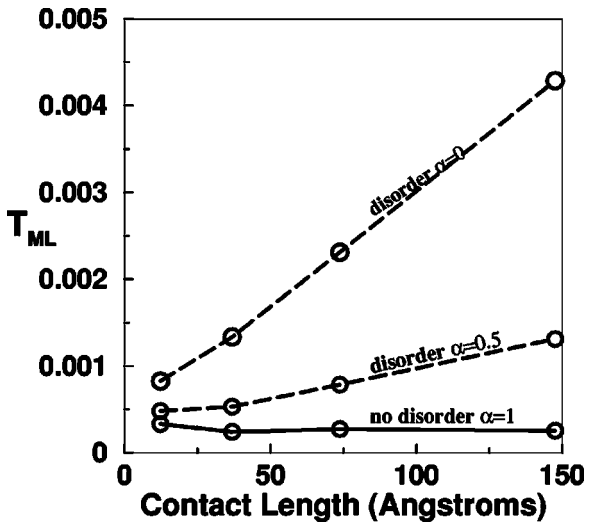

FIG. 5. Comparison of transmission probability vs the contact length for a (2,2) armchair tube, with and without disorder in nanotube-metal coupling. The metal Fermi wave vector is 0.75 Å^{-1}. Note that for the case without disorder, the transmission is poor, and increasing the contact length does not help. Introducing disorder changes this picture, and the transmission begins to increase with an increase in the contact length because **k**-vector conservation is relaxed.

and the conductance dependence on contact length are still valid. These features depend on nanotube-metal coupling along the axial direction. So any change due to the finite sector will not qualitatively change the results.

Experiments typically involve transmission of electrons between two metal contacts. The quantity T_{ML} discussed in this section, however, is the transmission probability between a metal contact and a semi-infinte nanotube (Fig. 2). We consider this quantity because a long nanotube section between two metal contacts requires much more numerically intensive calculations. The physics discussed with regards to T_{ML} in Figs. 3–5 also holds in the case of two metallic contacts, though a direct numerical comparison is not appropriate.

In the case of armchair tubes, when the metal Fermi wave vector k_f is smaller than $2\pi/3a_0$(0.85 Å^{-1}), T_{ML} does not change significantly with contact length, as shown for $k_f = 0.75$ Å^{-1} in Fig. 3(a). For values of k_f above the threshold, the transmission monotonically increases with an increase in the contact length. The monotonic increase is due to weak metal-nanotube coupling, in which case an increase in the contact length simply results in an increase in the transition probability to scatter from metal to nanotube [discussion surrounding Eqs. (1) and (2)].[15] The transmission will eventually saturate with an increase in the contact length, as there are only two conducting modes at the band center. For the configuration considered, T_{ML} can have a maximum value of unity. The second feature of Fig. 3(a) is the increase in transmission with an increase in k_f. This can be understood by noting that electrons with a wave-vector component along the nanotube axis that is larger than $2\pi/3a_0$ scatter from the metal to the nanotube, and a larger k_f implies a large number of available metal electron states. For the purpose of these calculations, we considered a (2,2) armchair tube. The essential physics would in principle also be true for the more realistic (10,10) nanotube.

The case of zigzag tubes is different because bands at $E = 0$ cross at $k = 0$. Then electrons in the metal electrode with any k_f (no threshold) can scatter into a metallic zigzag tube. The results for a (3,0) tube are shown in Fig. 3(b). Here there are two important points. The first point is that as there is no threshold metal Fermi wave vector, the transmission increases monotonically with the contact length even for $k_f = 0.4$ Å^{-1}, which is smaller than the threshold for armchair tubes. The second point is that the transmission for k_f equal to 1.2 Å^{-1} is much smaller than that for armchair tubes [Fig. 3(a); the transmissions of the three smaller values of k_f have been multiplied by a factor of 10]. This is because the nanotube wave vector around the circumference (k_c) of a zigzag tube is large, $k_c = 4\pi/3a_0$ for the crossing bands, and, as a result, the overlap integral [Eq. (1)] is smaller than for armchair tubes. $k_f = 1.2$ Å^{-1} is close to the Fermi wave vector for Au and Ag. As $k_f = 1.75$ Å^{-1} is larger than the threshold for graphite, the transmission probability is larger, and comparable to that for armchair tubes [Fig. 3(b)].

What happens when the diameter increases? In the limit of large diameter, a nanotube is akin to graphene, and to couple well with metal the threshold k_f should approach $4\pi/3a_0$.[10] Numerically, it is difficult to simulate large diameter tubes along with large contact lengths because of the time and memory requirements associated with the calcula-

tion of g_M^r. To convey the main point we consider two simpler cases. The first case compares the transmission probability of the two smallest semimetallic zigzag tubes with varying contact lengths, and the second case considers zigzag tubes of varying diameters with a rather small contact length. Figure 4 compares the transmission probability versus contact length of the (3,0) and (6,0) nanotubes. The (6,0) nanotube has twice the diameter of the (3,0) nanotube. The (6,0) nanotube correspondingly has a smaller transmission, and the trend of decrease in transmission will continue with further increase in the diameter. The inset is a calculation of the transmission probability versus the diameter of semimetallic zigzag tubes for a contact length of 42.6 Å (ten unit cells). T_{ML} decreases with an increase in the diameter, because wave-vector conservation becomes increasingly important with increase in the diameter. Also shown in this figure for comparison are 1/diameter and $1/\sqrt{\text{diameter}}$.

We now address the role of disorder. Disorder in either the nanotube, metal, or nanotube-metal coupling will in general result in larger transmission when compared to the disorder-free case. Wave-vector conservation is relaxed due to scattering from defects, and the transmission will increase with an increase in the contact length *even when the metal k_f is below the threshold value*. We consider the case of disorder in nanotube-metal coupling ($H_{c\text{-}m}$). Disorder in all elements of the coupling between the nanotube and metal is introduced randomly. The disorder in the coupling of atom i to the metal contact can be written as $t_i = \alpha t^{av} + (1-\alpha) t_i^{rand}$, where t^{av} is the average value of t_i over all sites connected to the metal, and α is a fraction between zero and unity. t_i^{rand} is the random component whose average is equal to t^{av}. In Fig. 5, the two strengths of disorder correspond to $\alpha = 0$ and 0.5 (the smaller α corresponds to larger disorder), such that t^{av} has the same value as in Fig. 3(a). For an armchair tube in contact with a metal with $k_f = 0.75$ Å^{-1}, the transmission is very small, and more importantly did not vary with contact length [Fig. 3(a)]. Introducing disorder changes this trend, and causes a monotonic increase in transmission with the length of contact [Fig. 5]. Similarly, for large diameter tubes, in the presence of disorder there should be significant transmission when k_f is smaller than the threshold $4\pi/3a_0$. The requirement of wave-vector conservation is also relaxed when the phase-coherence length is small. So we expect the coupling to improve with a decrease in the phase-coherence length.

IV. CONCLUSIONS

In this paper, we addressed some aspects of the physics of a nanotube side contacted to metal, a problem of current importance. The coupling of carbon nanotubes to metal depends on both chirality and diameter. Wave-vector conservation of an electron scattered from a nanotube to a metal plays a central role in determining the transport properties. The difference between small and large diameter nanotubes is that while in the former wave-vector conservation is important only in the axial direction, in the latter it is important in both the axial and circumferential directions. As a result, small diameter armchair and zigzag tubes have a cutoff value of the metal Fermi wave vector equal to $2\pi/3a_0$ and zero, respectively. For chiral tubes, the cutoff value of the metal Fermi wave vector lies in between these two limits, with the value decreasing with an increase in the chiral angle. A large diameter nanotube is akin to a graphene sheet, and the cutoff value of the metal Fermi wave vector in this case approaches $4\pi/3a_0$ with an increase in the diameter. Disorder in the metal, nanotube, or metal-nanotube coupling relaxes the requirement of **k**-vector conservation, and in general improves coupling. References 2 and 8 have shown an increase in conductance with contact length. In this paper, we discussed two situations that could lead to this. The first situation requires the metal Fermi wave vector to be larger than the threshold discussed in the text, and holds even when there is no disorder. The second situation requires disorder in coupling to the metal, but there is no restriction on the value of the Fermi wave vector.

Note added in proof. P. Delaney and M. Di Ventra [Appl. Phys. Lett. **75**, 4028 (2000)] also addresses the issue of wave vector conservation. We would like to thank M. Di Ventra for sending us a preprint.

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[14] One can also take the Fermi energy to lie off the band center, but this does not play an important role in conveying the main points of this paper.

[15] Note that if the nanotube-metal coupling is strong, then the transmission probability would reach its maximum by contacting only a few layers along the length. Further increase in the contact length will not result in a monotonic increase in transmission with contact length.